Quantum Systems

(Lecture 6: Quantum algorithms — Search problems and Grover)

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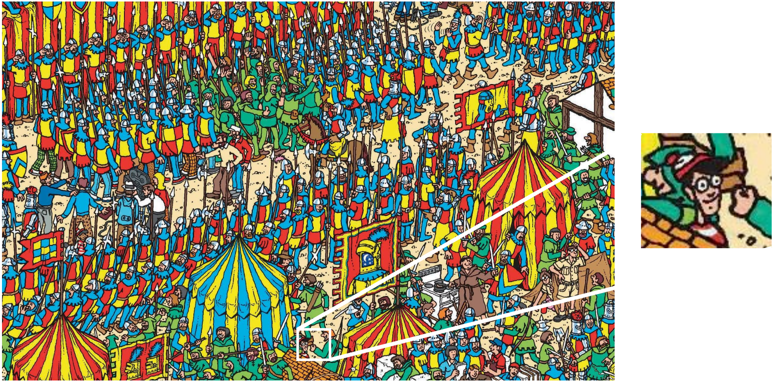
Search problems



Search problems

Search problem

- **Search space**: unstructured / unsorted
- **Asset**: a tool to efficiently recognise a solution

Example: Searching in a sorted vs unsorted database

- find a name in a telephone directory
- find a phone number in a telephone directory

Search problems

Note that a procedure to recognise a solution does not need to rely on a previous knowledge of it.

Example: password recognition

- $f(x) = 1 \quad \text{iff} \quad x = 123456789$ (f knows the password)
- $f(x) = 1 \quad \text{iff} \quad \mathit{hash}(x) = \text{c9b93f3f0682250b6cf8331b7ee68fd8}$
  (f recognises a correct password, but does not know it as inverting a hash function is, in general, very hard.)

Search problems

A typical formulation

Given a function $f : 2^n (= N) \longrightarrow 2$ such that there exists a unique number, encoded by a binary string a, st

$$f(x) = \begin{cases} 1 & \Leftarrow x = a \\ 0 & \Leftarrow x \neq a, \end{cases}$$

determine a.

A classical solution

- 0 evaluations of f: probability of success: $\frac{1}{2^n}$
- 1 evaluation of f: probability of success: $\frac{2}{2^n}$
  (choose a solution at random; if test fails choose another.)
- 2 evaluations of f: probability of success: $\frac{3}{2^n}$.
- k evaluations of f: probability of success: $\frac{k+1}{2^n}$.

Search problems

Grover's algorithm (1996)

Provides a quadratic speed up:

- Worst case for a classic algorithm: 2^n evaluations of f
- Worst case for Grover's algorithm: $\sqrt{2^n}$ evaluations of f

An oracle for f

... provides a means to recognize a solution for an input $|v\rangle$:

$$U_f \; = \; |v\rangle|t\rangle \mapsto |v\rangle|t \oplus f(v)\rangle$$

Thus, preparing the second (target) register with $|0\rangle$,

$$U_f \; = \; |v\rangle|0\rangle \mapsto |v\rangle|f(v)\rangle$$

Measuring the target after U_f will return its answer to the given input, as (classically) expected.

Superposition will make the difference to take advantage of quantum 'parallelism'.

$$\psi \; = \; \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle$$

An oracle for f

$|\psi\rangle$ can be expressed in terms of two states separating the solution states and the rest:

$$|a\rangle \text{ and } |r\rangle = \frac{1}{\sqrt{N-1}} \sum_{x \in N \setminus \{a\}} |x\rangle$$

which form a basis for a 2-dimensional subspace of the original N-dimensional space.

Thus,

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle = \underbrace{\frac{1}{\sqrt{N}}|a\rangle}_{\text{solution}} + \underbrace{\sqrt{\frac{N-1}{N}}|r\rangle}_{\text{the rest}}$$

An oracle for f

If the target qubit is set to $|-\rangle$, the effect of U_f is just

$$U_f \;=\; |x\rangle|-\rangle \mapsto (-1)^{f(x)}|x\rangle|-\rangle$$

This corresponds to a single qubit oracle which encodes the answer of U_f as a phase shift:

$$V \;=\; |x\rangle \mapsto (-1)^{f(x)}|x\rangle$$

$$\left(\text{i.e. } V|a\rangle = -|a\rangle \text{ and } V|x\rangle = |x\rangle \text{ (for } x \neq a) \right)$$

which can be expressed as

$$V \;=\; \sum_{x \neq a} |x\rangle\langle x| - |a\rangle\langle a| \;=\; I - 2|a\rangle\langle a|$$

An oracle for f

$$V = \sum_{x \neq a} |x\rangle\langle x| - |a\rangle\langle a| = I - 2|a\rangle\langle a| = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & -1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\ & & & \cdots & & & \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

V identifies the solution but does not allow for an observer to retrieve it because the square of the amplitudes for any value is always $\frac{1}{N}$.

An amplifier

This entails the need for a mechanism to boost the probability of retrieving the solution.

$$
\begin{aligned}
P &= |x\rangle \mapsto (-1)^{\delta_{x,0}} |x\rangle \\
&= |0\rangle\langle 0| + (-1) \sum_{x \neq 0} |x\rangle\langle x| \\
&= |0\rangle\langle 0| + (-1)(I - |0\rangle\langle 0|) \\
&= 2|0\rangle\langle 0| - I
\end{aligned}
$$

P applies a phase shift to all vectors in the subspace spanned by all the basis states $|x\rangle$, for $x \neq 0$.

An amplifier

Recall our input state

$$|\psi\rangle = H^{\otimes n}|00\cdots 0\rangle = |+\rangle^{\otimes n} = \frac{1}{\sqrt{N}}\sum_{x=0}^{N-1}|x\rangle$$

and define an operator $W = H^{\otimes n}\, P\, H^{\otimes n}$, which

- $W|\psi\rangle = |\psi\rangle$,
- $W|\phi\rangle = -|\phi\rangle$, for any vector $|\phi\rangle$ in the subspace orthogonal to $|\psi\rangle$ (i.e. spanned by the basis vectors $H|x\rangle$ for $x \neq 0$).

$$\begin{aligned} W &= H^{\otimes n}\, P\, H^{\otimes n} \\ &= H^{\otimes n}\,(2|0\rangle\langle 0| - I)\, H^{\otimes n} \\ &= 2(H^{\otimes n}|0\rangle\langle 0|H^{\otimes n}) - H^{\otimes n}\, I\, H^{\otimes n} \\ &= 2|\psi\rangle\langle\psi| - I \end{aligned}$$

The effect of W: to *invert about the mean*

$$
\begin{aligned}
W\left(\sum_k \alpha_k |k\rangle\right) &= \left(2\left(\frac{1}{\sqrt{N}}\sum_{x=0}^{N-1}|x\rangle \frac{1}{\sqrt{N}}\sum_{y=0}^{N-1}\langle y|\right) - I\right)\sum_k \alpha_k|k\rangle \\
&= \left(2\left(\frac{1}{N}\sum_{x=0}^{N-1}|x\rangle \sum_{y=0}^{N-1}\langle y|\right) - I\right)\sum_k \alpha_k|k\rangle \\
&= 2\left(\frac{1}{N}\sum_{x,y,k}\alpha_k|x\rangle\langle y|k\rangle\right) - \sum_k \alpha_k|k\rangle \\
&= 2\left(\underbrace{\frac{1}{N}\sum_k \alpha_k}_{\alpha\text{ - mean}}\sum_x |x\rangle\right) - \sum_k \alpha_k|k\rangle \\
&= 2\,\alpha\sum_k |k\rangle - \sum_k \alpha_k|k\rangle \\
&= \sum_k (2\,\alpha - \alpha_k)|k\rangle
\end{aligned}
$$

Invert about the mean: Example

The mean:

$$\Big(\frac{1}{3}\sum_{x=0}^{2}|x\rangle\sum_{y=0}^{2}\langle y|\Big)\overbrace{\begin{bmatrix}2\\-2\\2\end{bmatrix}}^{\sum_k \alpha_k|k\rangle} = \frac{1}{3}\begin{bmatrix}1&1&1\\1&1&1\\1&1&1\end{bmatrix}\overbrace{\begin{bmatrix}2\\-2\\2\end{bmatrix}}^{\sum_k \alpha_k|k\rangle} = \frac{1}{3}\begin{bmatrix}2\\2\\2\end{bmatrix} = \overbrace{\begin{bmatrix}\frac{2}{3}\\\frac{2}{3}\\\frac{2}{3}\end{bmatrix}}^{\alpha\sum_k|k\rangle}$$

The new state:

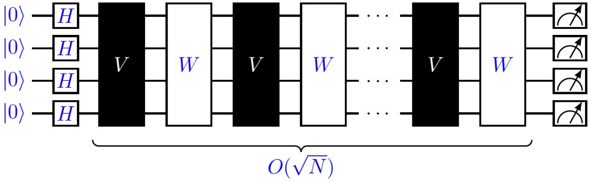
$$2\overbrace{\begin{bmatrix}\frac{2}{3}\\\frac{2}{3}\\\frac{2}{3}\end{bmatrix}}^{\alpha\sum_k|k\rangle} - \overbrace{\begin{bmatrix}2\\-2\\2\end{bmatrix}}^{\sum_k \alpha_k|k\rangle} = \begin{bmatrix}\frac{4}{3}-2\\\frac{4}{3}+4\\\frac{4}{3}-2\end{bmatrix} = \begin{bmatrix}-\frac{2}{3}\\\frac{16}{3}\\-\frac{2}{3}\end{bmatrix}$$

$\boxed{W \text{ inverts and boosts the right amplitude; slightly reduces the others.}}$

The Grover iterator

$$
\begin{aligned}
G &= WV \\
&= H^{\otimes n} \, P \, H^{\otimes n} \, V \\
&= (2|\psi\rangle\langle\psi| - I)\,(I - 2|a\rangle\langle a|)
\end{aligned}
$$

The Grover circuit



The Grover iterator

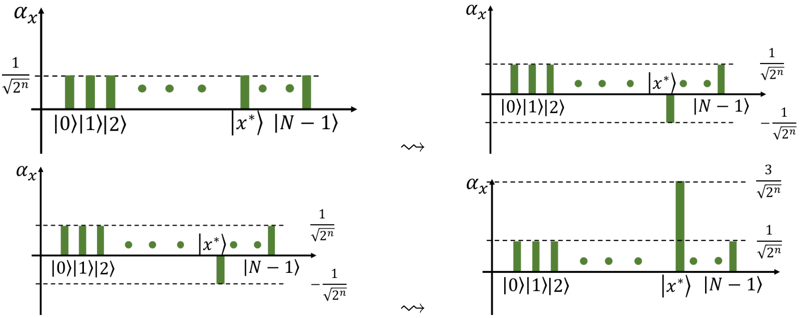
Example

- Start with $[10, 10, 10, 10, 10]^T$
- Invert the fourth entry: $[10, 10, 10, -10, 10]^T$
- Invert around mean (6): $[2, 2, 2, 22, 2]^T$
  Note $12 - (-10) = 22$
- Invert the fourth entry again: $[2, 2, 2, -22, 2]^T$
- Invert around mean (-2.8): $[-7.6, -7.6, -7.6, 16.4, -7.6]^T$
  Note $2 * (-2.8) - (-22) = 16.4$.
- ...

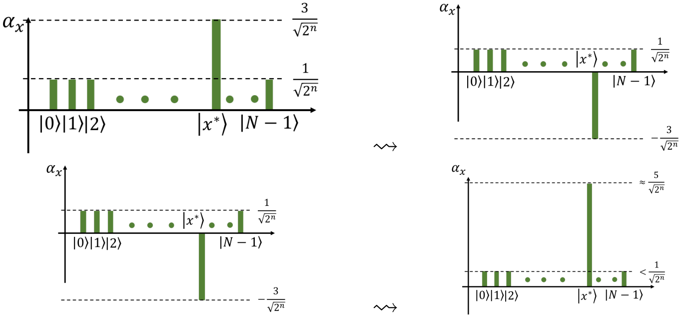
The phase corresponding to the solution is amplified in successive iterations

The Grover iterator

As $H^{\otimes n}|00\cdots 0\rangle$ has real amplitudes and G does not introduce complex phases, amplitudes remain real and can, thus, be depicted as vertical lines around an axis representing all possible inputs



The Grover iterator



A geometric perspective on G

Initial state: $|\psi\rangle = \frac{1}{\sqrt{N}}|a\rangle + \sqrt{\frac{N-1}{N}}|r\rangle$

The repeated application of G leaves the system in the 2-dimensional subspace of the original N-dimensional space, spanned by $|a\rangle$ and $|r\rangle$.

Another basis is given by $|\phi\rangle$ and the state orthogonal to $|\phi\rangle$:

$$|\overline{\psi}\rangle = -\frac{1}{\sqrt{N}}|a\rangle + \sqrt{\frac{N-1}{N}}|r\rangle$$

Define an angle θ st $\sin\theta = \frac{1}{\sqrt{N}}$ (and, of course, $\cos\theta = \sqrt{\frac{N-1}{N}}$), and express the two basis as

$$|\psi\rangle = \sin\theta|a\rangle + \cos\theta|r\rangle \quad |\overline{\psi}\rangle = \cos\theta|a\rangle - \sin\theta|r\rangle$$

$$|a\rangle = \sin\theta|\psi\rangle + \cos\theta|\overline{\psi}\rangle \quad |r\rangle = \cos\theta|\psi\rangle - \sin\theta|\overline{\psi}\rangle$$

A geometric perspective on G

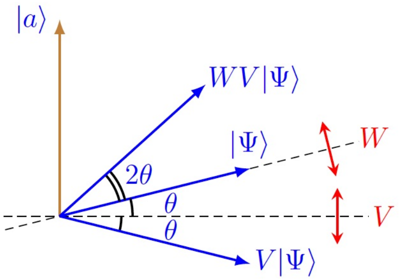
$$
\begin{aligned}
V|\psi\rangle &= -\sin\theta|a\rangle + \cos\theta|r\rangle \\
&= -\sin\theta(\sin\theta|\psi\rangle + \cos\theta|\overline{\psi}\rangle) + \cos\theta(\cos\theta|\psi\rangle - \sin\theta|\overline{\psi}\rangle) \\
&= -\sin^2\theta|\psi\rangle - \sin\theta\cos\theta|\overline{\psi}\rangle + \cos^2\theta|\psi\rangle - \cos\theta\sin\theta|\overline{\psi}\rangle \\
&= (-\sin^2\theta + \cos^2\theta)|\psi\rangle - 2\sin\theta\cos\theta|\overline{\psi}\rangle \\
&= \cos 2\theta|\psi\rangle - \sin 2\theta|\overline{\psi}\rangle
\end{aligned}
$$

and

$$
G|\psi\rangle = \cos 2\theta|\psi\rangle + \sin 2\theta|\overline{\psi}\rangle
$$

The effect of G is a 2θ rotation

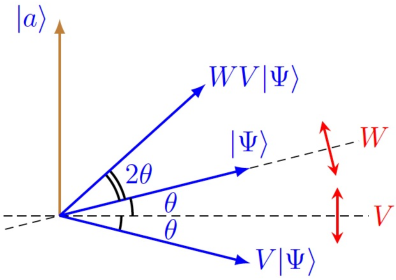
A geometric perspective on G



- $V|a\rangle = -|a\rangle$, i.e. a reflection over $|r\rangle$,
- $W|\psi\rangle = |\psi\rangle$, i.e. a reflection over $|\psi\rangle$

Thus, as a combination of two reflections, the effect of G is a 2θ rotation.

A geometric perspective on G



From this picture, we may also conclude that

- the angular distance to cover $=$ $\arccos \frac{1}{\sqrt{N}} = \frac{\pi}{2} - \theta$, clearly $\leq \frac{\pi}{2}$,
- and $\sin \theta = \cos(\frac{\pi}{2} - \theta) = \langle a|\psi\rangle = \frac{1}{\sqrt{N}}$
  (because $\langle u|v\rangle = \| |u\rangle \| \, \| |v\rangle \| \cos\theta$)

How many times should G be applied?

Thus, the ideal number of iterations is

$$t = \left\lfloor \frac{\arccos \frac{1}{\sqrt{N}}}{2\theta} \right\rfloor$$

A lower bound for θ gives an upper bound for t
— for N large $\theta \approx \sin\theta = \frac{1}{\sqrt{N}}$. Thus,

$$t \approx \frac{\pi}{4}\sqrt{N}$$

So, G applied t times leaves the system within an angle θ of $|a\rangle$. Then, a measurement in the computational basis yields the correct solution with probability

$$\| \langle a|G^t|\psi\rangle \| \geq \cos^2\theta = 1 - \sin^2\theta = \frac{N-1}{N}$$

which, for large N, is very close to 1.

How many times should G be applied?

For an alternative computation, recall

$$G|\psi\rangle = \cos 2\theta|\psi\rangle + \sin 2\theta|\overline{\psi}\rangle$$

By induction, after k iterations,

$$\begin{aligned} G^k|\psi\rangle &= \cos(2k\theta)|\psi\rangle + \sin(2k\theta)|\overline{\psi}\rangle \\ &= \sin(2k+1)\theta|a\rangle + \cos(2k+1)\theta|r\rangle \end{aligned}$$

Thus, to maximize the probability of obtaining $|a\rangle$, k is selected st

$$\sin((2k+1)\theta) \approx 1 \quad \text{i.e.} \quad (2k+1)\theta \approx \frac{\pi}{2}$$

which leads to

$$k \approx \frac{\pi}{4\theta} - \frac{1}{2} \approx \frac{\pi}{4}\sqrt{N} \approx t$$

Grover's algorithm ($\mathcal{O}(\sqrt{N})$)

- Prepare the initial state: $|0\rangle^{\otimes n}|1\rangle$
- Apply $H^{\otimes n} \otimes H$ to yield $\frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle|-\rangle$
- Apply the Grover iterator G to $\frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle|-\rangle$, $t \approx \frac{\pi}{4}\sqrt{N}$ times, leading approximately to state $|a\rangle|-\rangle$
- Measure the first n qubits to retrieve $|a\rangle$

Multiple solutions

$\boxed{\text{There } M \text{ (out of } 2^n = N\text{) input strings evaluating to 0 by } f}$

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle = \underbrace{\sqrt{\frac{M}{N}}|s\rangle}_{\text{solution}} + \underbrace{\sqrt{\frac{N-M}{N}}|r\rangle}_{\text{the rest}}$$

where

$$|s\rangle = \frac{1}{\sqrt{M}} \sum_{x \text{ solution}} |x\rangle \quad \text{and} \quad |r\rangle = \frac{1}{\sqrt{N-M}} \sum_{x \text{ no solution}} |x\rangle$$

Multiple solutions

$$t = \left\lfloor \frac{\arccos \sqrt{\frac{M}{N}}}{2\theta} \right\rfloor$$

which, for N large, $M \ll N$ (thus $\theta \approx \sin\theta$), yields

$$t \approx \frac{\pi}{4}\sqrt{\frac{N}{M}}$$

The probability to retrieve a correct solution is

$$\| \langle s|G^t|\psi\rangle \| \geq \cos^2\theta = 1 - \sin^2\theta = \frac{N-M}{N}$$

which, for $M = \frac{N}{2}$ yields $\frac{1}{2}$, but for $M \ll N$, is again close to 1.

Multiple solutions

Computing the effect of G: 2θ

$$\sin 2\theta = 2\sqrt{\frac{N-M}{N}} = 2\frac{\sqrt{M(N-M)}}{N}$$

$$2\theta = \arcsin(2\frac{\sqrt{M(N-M)}}{N})$$

M (out of 100)	$\arcsin\theta$
0	0
1	0.198
20	0.8
40	0.979
50	1
60	0.979
80	0.8
99	0.198
M	0

Multiple solutions

Surprisingly, the rotation in each iteration decreases from $M = \frac{N}{2}$ to N, and the number of iterations consequently increases, although one would expect to be easier to find a correct solution if their number increases!

Solution

To double the number of elements in the search space, by adding N extra elements, none of which being a solution.

The technique: Phase amplification

Grover's algorithm made use of

$$H^{\otimes n}|00\cdots 0\rangle$$

to prepare a uniform superposition of potential solutions. The same module was used for phase amplification inside G.

In general, one may resort to any module K to map the solution space to any superposition of guesses, plus some extra qubits to be used as draft paper:

$$K|00\cdots 0\rangle \;=\; \sum_x \alpha_x|x\rangle\,|\mathrm{draft}(x)\rangle$$

The technique: Phase amplification

$$|\psi\rangle = \sum_{x \text{ solution}} \alpha_x |x\rangle\, |\mathrm{draft}(x)\rangle + \sum_{x \text{ no solution}} \alpha_x |x\rangle\, |\mathrm{draft}(x)\rangle$$

yielding the following probabilities:

$$p_s = \sum_{x \text{ solution}} \| \alpha_x \|^2 \quad \text{and} \quad p_{ns} = \sum_{x \text{ no solution}} \| \alpha_x \|^2 = 1 - p_s$$

Of course, amplification has no use if $p_s \in \{0, 1\}$.

The technique: Phase amplification

Otherwise ($0 < p_s < 1$), the phases of solution inputs should be amplified.
First, express

$$|\psi\rangle \;=\; \sqrt{p_s}|\psi_s\rangle \;+\; \sqrt{p_{ns}}|\psi_{ns}\rangle$$

for the normalised components

$$|\psi_s\rangle \;=\; \sum_{x\ \text{solution}} \frac{\alpha_x}{\sqrt{p_s}}|x\rangle\,|\text{draft}(x)\rangle$$

$$|\psi_{ns}\rangle \;=\; \sum_{x\ \text{solution}} \frac{\alpha_x}{\sqrt{p_{ns}}}|x\rangle\,|\text{draft}(x)\rangle$$

which rewrites to

$$|\psi\rangle \;=\; \sin\theta|\psi_s\rangle \;+\; \cos\theta|\psi_{ns}\rangle$$

for $\theta \in \{0, \frac{\pi}{2}\}$ such that $\sin^2\theta = p_s$.

The technique: Phase amplification

A generic search iterator is built as

$$S = KPK^{-1}V = W_K V$$

where

$$W_K|\psi\rangle = |\psi\rangle$$
$$W_K|\phi\rangle = -|\phi\rangle \quad \text{for all states orthogonal to } |\psi\rangle$$

The technique: Phase amplification

The repeated application of S a total of k times rotates the initial state $|\psi\rangle$ to

$$S^k|\psi\rangle = \sin((2k+1)\theta)|\psi_s\rangle + \cos((2k+1)\theta)|\psi_{ns}\rangle$$

For the correct number of iterations, this procedure reaches a state such that a measurement will return an element of the subspace spanned by $|\psi_s\rangle$ with a probability close to 1.

The technique: Phase amplification

As before, to get that high probability, the smallest value for k one can choose is such that

$$(2k+1)\theta \approx \frac{\pi}{2}$$

which implies $k \in \mathcal{O}(\frac{1}{\theta})$.

For a small θ, as

$$\sin\theta = \sqrt{p_s} \approx \theta$$

the magnitude of the right number of iterations is

$$\mathcal{O}\left(\sqrt{\frac{1}{\theta}}\right)$$

Quantum algorithms

Recall the generic idea: engineering quantum effects as computational resources

Classes of algorithms

- Algorithms with superpolynomial speed-up, typically based on the quantum Fourier transform, include Shor's algorithm for prime factorization. The level of resources (qubits) required is not yet currently available.
- Algorithms with quadratic speed-up, typically based on amplitude amplification, as in the variants of Grover's algorithm for unstructured search. Easier to implement in current NISQ technology, typical component of other algorithms.
- Quantum simulation — not covered in this course.

... and we are done!

What have we covered

- Reactive systems:
  - classical interaction (communication)
  - + programmed parallelism (operators, e.g. $|$)
  - + engineering
- Quantum systems:
  - quantum interaction (entanglement)
  - + physical/natural parallelism (superposition)
  - + engineering

... and we are done!

Where to look further

- Reactive computation is the base of the everyware — namely in its extensions to hybrid (discrete-continuous) programming and cyber-physical systems.
  Covered in the Formal Methods profile in the MSc on Informatics Engineering.

- Quantum computation is an extremely young and challenging area, looking for young people either with a theoretic or experimental profile.
  Get in touch if you are interested in pursuing studies/research in the area at UMinho, INESC TEC and INL.

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